Sulfachloropyridazine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.41

Global applicability domain: Inside

Local applicability domain index: 3.09e-01

Confidence level: 7.08e-01

Nearest Neighbors from the Training Set

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Dichlorvos
Measured: 5.01e-01
Predicted: 6.47e-01

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Triethyl phosphate
Measured: 1.29
Predicted: 1.38

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Tris(2-chloroethyl) phosphate
Measured: 1.29
Predicted: 1.66

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Triallyl phosphate
Measured: 1.20
Predicted: 1.41

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Tris(2-chloroisopropyl)phosphate
Measured: 7.94
Predicted: 6.64